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Numerical simulation of a quantum controlled-not gate implemented on four-spin molecules at room temperature

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Abstract

We study numerically the non-resonant effects on four-spin molecules at room temperature with the implemented quantum controlled-not gate and using the $2\pi k$ method. The four nuclear spins in each molecule represent a four-qubit register. The qubits interact with each other through Ising-type interaction which is characterized by the coupling constant $J_{a,b}$. We study the errors on the reduced density matrix as a function of the Rabi frequency, Ω , using the $2\pi k$ method and when all the coupling constants are equal or when one of them is different from the others.

Keywords: Quantum computing, quantum communication, controlled-not gate

1. Introduction

Instead of bits with values of '0' and '1' used in classical computers, a quantum computer uses quantum bits, called qubits, represented by a superposition of two basic states $|0\rangle$ and $|1\rangle$ ([1–16]): $\Psi = c_1|0\rangle + c_2|1\rangle$ such as $|c_1|^2 + |c_2|^2 = 1$. For a molecule containing four nuclear spins (qubits) which we shall label '0', '1', '2' and '3', from right to left, one has the state

$$\Psi = c_0|0_3 0_2 0_1 0_0\rangle + c_1|0_3 0_2 0_1 1_0\rangle + \dots + c_{15}|1_3 1_2 1_1 1_0\rangle, \quad (1a)$$

where

$$\sum_{k=0}^{15} |c_k|^2 = 1 \quad (1b)$$

and the c_k are time-dependent coefficients. The first quantum computation has been demonstrated using nuclear magnetic resonance (NMR) techniques at room temperature [17]. One of the most important aspects of dynamics is the influence of non-resonant interactions. To understand the dynamics arising from the time-dependent Hamiltonian (H), which describes the interaction of the molecules with the electromagnetic field and the coupling among the spins, one need to be aware of the

non-resonant effects. The first quantum computation at room temperature was accomplished using NMR techniques [17]. After this, it was realized that one of the most important aspects of the dynamics is the influence of non-resonant interactions. This is especially true for the study of the dynamics arising from the time-dependent H , which describes the interaction of the molecules with the electromagnetic field and the coupling among the spins.

In our previous paper [18] we studied numerically the influence of non-resonant effects on the dynamics of a single π -pulse quantum controlled-not (CN) gate in an ensemble of four-spin molecules at room temperature, where the interaction among the spins was assumed to be of the Ising type. We also studied the region of parameters in which a single-pulse quantum CN gate can be implemented at room temperature (NMR). After finding a method to suppress the non-resonant effects on nuclear spin-1/2 systems [19, 20], the so-called ' $2\pi k$ method', which consists of selecting the value of the Rabi frequency (Ω_a) in such a way that the unwanted transitions among levels in the system are suppressed, the question arises about whether or not this method [19] can be equally effective on four-spin molecules at room temperature. In this paper, we study numerically the effect of the $2\pi k$

method on the performance of the CN gate in an ensemble of four-spin molecules at room temperature. The paper is organized as follows. The dynamics of the system is established in section 2. The quantum CN gate and selection of the Rabi frequency using the $2\pi k$ method are explained in section 3. The numerical results obtained with the simulations are presented in section 4. Finally, in section 5 we summarize our results.

2. Dynamics

Consider an ensemble of four-spin molecules at room temperature interacting with the electromagnetic field

$$\mathbf{B} = (B_t \cos \omega t, -B_t \sin \omega t, B_z), \quad (2)$$

where B_t is the amplitude of the circularly polarized magnetic field which rotates in the (x, y) plane with frequency ω , and B_z is the z -component of the magnetic field. All spins interact with each other through the Ising interaction with the constants $J_{\alpha,\beta}$ ($\alpha, \beta = 0, 1, 2, 3$). The H of the system is $H = H_o + V$, where H_o and V are given by

$$H_o = -\hbar \sum_{\alpha=0}^3 \left[\omega_{\alpha} I_{\alpha}^z + 2 \sum_{\beta>\alpha} J_{\alpha,\beta} I_{\alpha}^z I_{\beta}^z \right] \quad (3)$$

and

$$V = -\frac{\hbar}{2} \sum_{\alpha=0}^3 \Omega_{\alpha} (e^{i\omega t} I_{\alpha}^+ + e^{-i\omega t} I_{\alpha}^-) \quad (4)$$

where $\omega_{\alpha} = \gamma_{\alpha} B_z$ is the frequency of the spin precession due to Zeeman interaction (γ_{α} is the gyromagnetic ratio), $\Omega_{\alpha} = \gamma_{\alpha} B_t$ is the Rabi frequency and $I_{\alpha}^{\pm} = I_{\alpha}^x \pm iI_{\alpha}^y$, where $I_{\alpha}^{x,y,z}$ is related to the Pauli matrix $\sigma_{\alpha}^{x,y,z}$ by $I_{\alpha}^{x,y,z} = \sigma_{\alpha}^{x,y,z}/2$. The term $J_{\alpha,\beta}$ is the coupling constant of interaction between the α spin and β spin of the molecule. This H represents a very good approximation to the realistic situation [21] and it is used to solve the equation for the density matrix: $i\hbar(d\rho/dt) = [H, \rho]$. The Hamiltonian H is time dependent. This time dependence can be eliminated by transforming it to a system of coordinates that rotates with the frequency of the external magnetic field, ω . On this rotating system of coordinates, H is given [17] by

$$\bar{H} = U_{\omega}^{\dagger} H U_{\omega} = H' + V', \quad (5a)$$

$$H' = -\hbar \sum_{\alpha=0}^3 \left[(\omega_{\alpha} - \omega) I_{\alpha}^z + 2 \sum_{\beta>\alpha} J_{\alpha,\beta} I_{\alpha}^z I_{\beta}^z \right], \quad (5b)$$

$$V' = -\hbar \sum_{\alpha=0}^3 \Omega_{\alpha} I_{\alpha}^x, \quad (5c)$$

where U_{ω} is the unitary operator defined as

$$U_{\omega} = \exp \left[i\omega t \left(\sum_{\alpha=0}^3 I_{\alpha}^z \right) \right]. \quad (5d)$$

The equation for the new density matrix, $\rho' = U_{\omega}^{\dagger} \rho U_{\omega}$, is: $i\hbar(d\rho'/dt) = [\bar{H}, \rho']$. On this rotating system of coordinates and using the complete set of basis states, $|i_3 i_2 i_1 i_0\rangle$, $i_j = 0, 1$

for $j = 0, 1, 2, 3$, the energies of the ground state, $|0000\rangle$, and the first excited state, $|0001\rangle$, are given by

$$E'_0 = -\frac{\hbar}{2} \sum_{\alpha=0}^3 \left[(\omega_{\alpha} - \omega) + \sum_{\beta>\alpha} J_{\alpha,\beta} \right] \quad (6a)$$

and

$$E'_1 = -\frac{\hbar}{2} (-\omega_0 + \omega_1 + \omega_2 + \omega_3 - 2\omega - J_{0,1} - J_{0,2} - J_{0,3} + J_{1,2} + J_{1,3} + J_{2,3}). \quad (6b)$$

In spite of the fact that the equation for the density matrix, ρ' , has time-independent coefficients, this equation is still not convenient for numerical calculations. This equation includes both fast and slow dynamics. Fast dynamics is associated with the presence of high-frequency terms $\sim(\omega_{\alpha} - \omega)$, while slow dynamics is associated with terms proportional to the Rabi frequency, $\sim\Omega_{\alpha} \ll \omega_{\alpha}$. For numerical calculation of the density matrix, it is convenient to exclude high-frequency oscillations for each qubit. To do this, we use the unitary transformation $U_t = \exp(-iH't/\hbar)$. Then we have the following equation for the new density matrix:

$$i\hbar \frac{d\tilde{\rho}}{dt} = [\tilde{V}, \tilde{\rho}], \quad (\tilde{\rho} = U_t^{\dagger} \rho' U_t, \tilde{V} = U_t^{\dagger} V' U_t). \quad (7)$$

In addition, if E_k , $k = 0, \dots, 15$, are the eigenvalues of H (equation 3), the condition $E_k/k_B T \ll 1$ (where k_B is the Boltzmann constant and T is the temperature) is satisfied, and it is possible to write the density matrix as [1, 17, 18]

$$\tilde{\rho} = E/16 + \rho_{\Delta}, \quad (8)$$

where E is the identity matrix and ρ_{Δ} has the property $\text{tr } \rho_{\Delta} = 0$ and can be expressed as

$$\rho_{\Delta}(t) = \frac{\hbar \sum_{k=0}^3 \omega_k}{32k_B T} \sum_{n,k=0}^{15} r_{n,k}(t) |n\rangle \langle k|, \quad (9)$$

with the initial condition,

$$r(0) = \sum_{n,k} r_{n,k}(0) |n\rangle \langle k| + \frac{1}{2} \{ -|4\rangle \langle 4| + |5\rangle \langle 5| + |6\rangle \langle 6| + |7\rangle \langle 7| + |8\rangle \langle 8| - |9\rangle \langle 9| - |10\rangle \langle 10| - |11\rangle \langle 11| - |12\rangle \langle 12| \} \quad (10a)$$

where $r_{n,k}(0)$ are called reduced density matrix elements and are written in term of the coefficients of pure two-spin system as

$$r_{n,k}(0) = c_n(0) c_k^*(0), \quad n, k = 0, 1, 2, 3. \quad (10b)$$

The idea suggested in [7] was to use the first four basic elements $|00kl\rangle$ ($k, l = 0, 1$) as the 'active states' for quantum logic operation. So, the dynamics of the four-spin molecules is similar to the dynamics of a pure quantum system of two interacting spins. The initial states used for our study are

$$\Psi_a = \sqrt{0.3} |0000\rangle + \sqrt{0.2} |0001\rangle + \frac{1}{\sqrt{3}} |0010\rangle + \frac{1}{\sqrt{6}} |0011\rangle \quad (11a)$$

$$\Psi_b = \frac{1}{2} (|0000\rangle + |0001\rangle + |0010\rangle + |0011\rangle) \quad (11b)$$

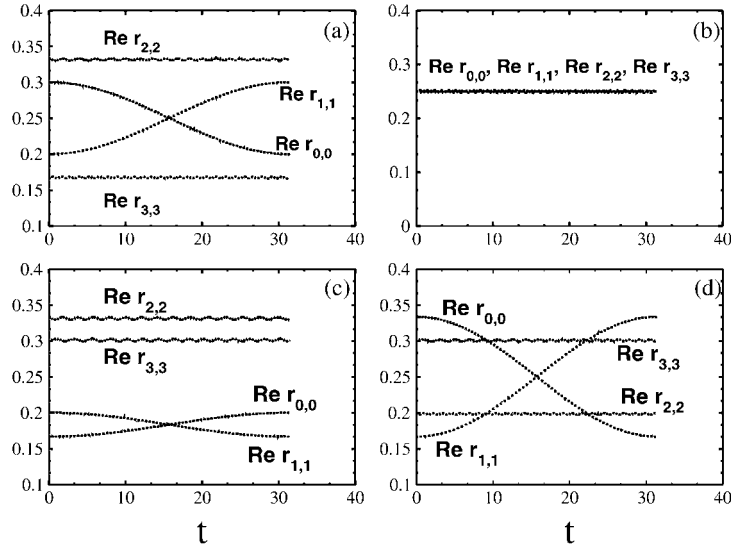


Figure 1. Evolution of the first four diagonal elements (real part) of the reduced density matrix under the action of a π -pulse and for the four initial conditions defined by the wavefunctions (11 *a, b, c, d*).

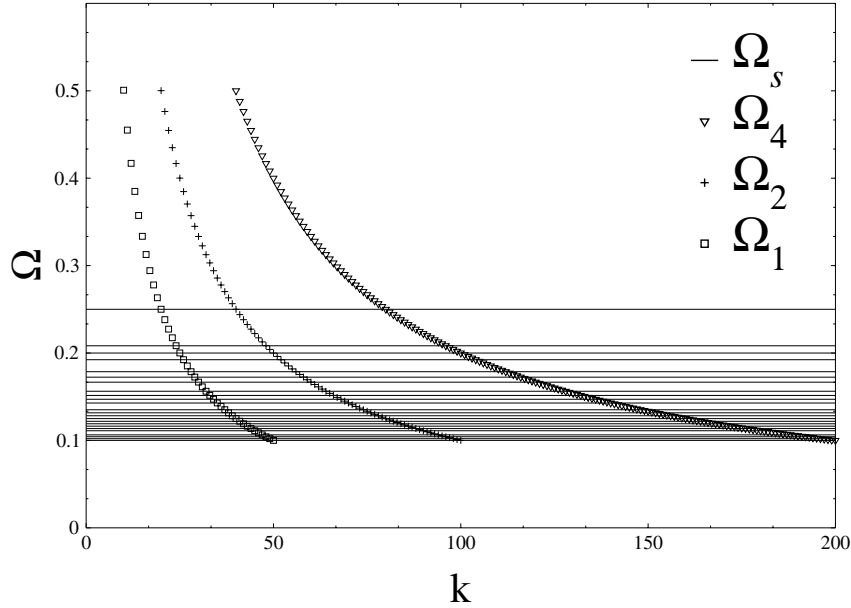


Figure 2. Variation of Ω_1 , Ω_2 and Ω_4 with respect to k . Ω_s values are shown as horizontal lines for which one has $\Omega_s = \Omega_1 = \Omega_2 = \Omega_4$ for some different k values.

$$\Psi_c = \frac{1}{\sqrt{6}}|0000\rangle + \sqrt{0.2}|0001\rangle + \frac{1}{\sqrt{3}}|0010\rangle + \sqrt{0.3}|0011\rangle \quad (11c)$$

$$\Psi_d = \frac{1}{\sqrt{6}}|0000\rangle + \frac{1}{\sqrt{3}}|0001\rangle + \sqrt{0.2}|0010\rangle + \sqrt{0.3}|0011\rangle \quad (11d)$$

3. Quantum CN gate

The implementation of a quantum CN gate in the ensemble of four-spin molecules at room temperature is given by

$$\widehat{CN} = i|0000\rangle\langle 0001| + i|0001\rangle\langle 0000| + \sum_{p,q,r,s=0,1} |pqrs\rangle\langle pqrs| \quad (12)$$

where $|pqrs\rangle \neq |0000\rangle, |0001\rangle$. This operator changes the state of the right-most spin (target) only if its neighbour (control) spin is in the '0' state. The phase 'i' in this expression appears in natural way in our system [18, 20] and represents a generalization of the pure CN gate. This phase depends on the parameters $J_{\alpha,\beta}$ and ω_α which can be selected to get a pure CN gate. For the \widehat{CN} gate to work like a \widehat{CN} gate for pure quantum two-spin system at the end of the π -pulse ($\tau = \pi/\Omega$) the following relation must exist between the initially reduced density matrix, $r(0)$, and the final one, $r(\tau)$

$$\begin{bmatrix} r_{00}(\tau) & r_{01}(\tau) & r_{02}(\tau) & r_{03}(\tau) \\ r_{10}(\tau) & r_{11}(\tau) & r_{12}(\tau) & r_{13}(\tau) \\ r_{20}(\tau) & r_{21}(\tau) & r_{22}(\tau) & r_{23}(\tau) \\ r_{30}(\tau) & r_{31}(\tau) & r_{32}(\tau) & r_{33}(\tau) \end{bmatrix}$$

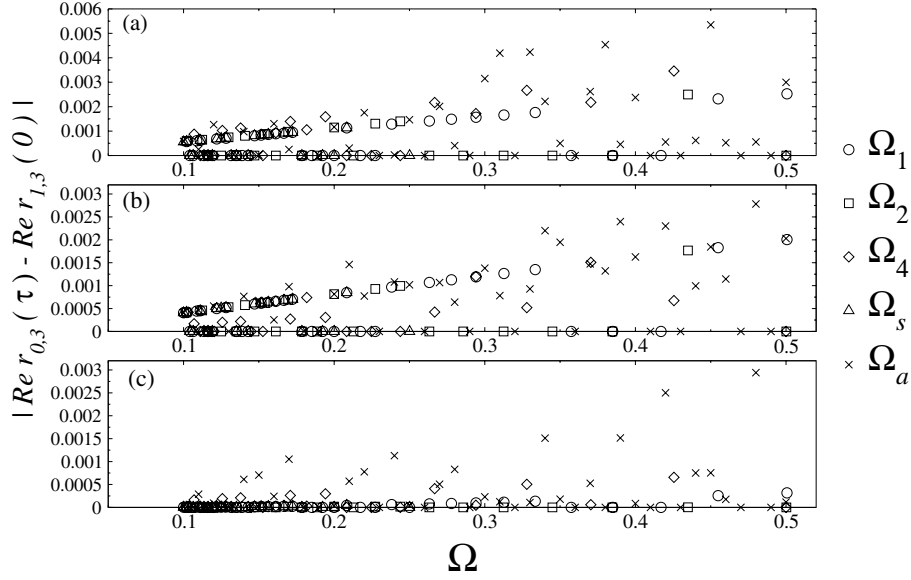


Figure 3. Error at the end of the π -pulse on $\text{Re } r_{0,3}(\tau)$ as a function of the Rabi frequency Ω , where Ω_a is an arbitrary Ω ; Ω_1 , Ω_2 and Ω_4 defined by (15); and Ω_s is given as shown on figure 2. (a) Represents the case $J = 10$; (b) represents the case $V_{2,3} = 0$; and (c) represents the case $J = 10$, $J' = 20$ and $V_{2,3} \neq 0$.

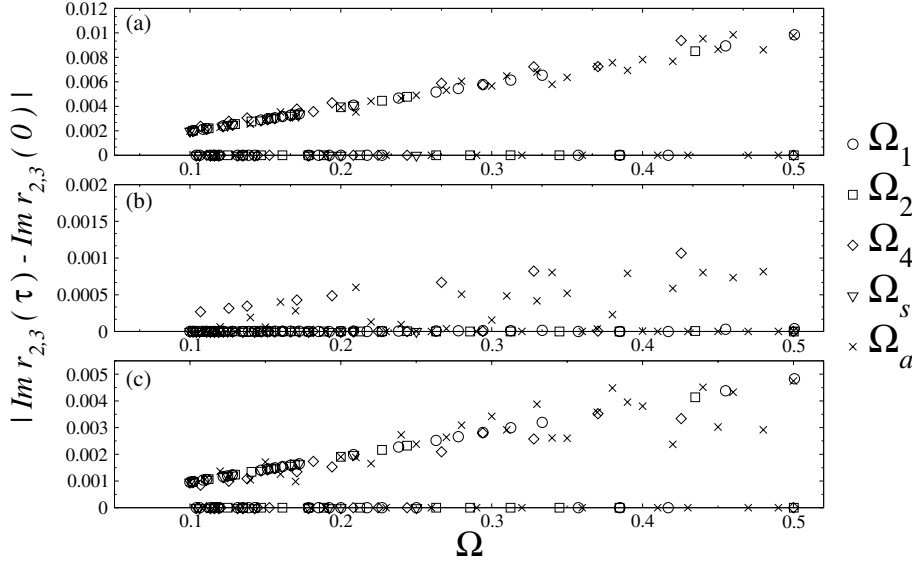


Figure 4. Error at the end of the π -pulse on $\text{Im } r_{0,3}(\tau)$ as a function of the Rabi frequency Ω , where Ω_a is an arbitrary omega; Ω_1 , Ω_2 and Ω_4 defined by (15); and Ω_s is given as shown on figure 2. (a) Represents the case $J = 10$; (b) represents the case $V_{2,3} = 0$; and (c) represents the case $J = 10$, $J' = 20$ and $V_{2,3} \neq 0$.

$$= \begin{bmatrix} r_{11}(0) & r_{10}(0) & ir_{12}(0) & ir_{13}(0) \\ r_{01}(0) & r_{00}(0) & ir_{02}(0) & ir_{03}(0) \\ -ir_{21}(0) & -ir_{20}(0) & r_{22}(0) & r_{23}(0) \\ -ir_{31}(0) & -ir_{30}(0) & r_{32}(0) & r_{33}(0) \end{bmatrix}. \quad (13)$$

Of course, this means that after four π -pulses one comes back to the initial density matrix. None of the other reduced matrix elements change significantly under this operation. For our numerical study, we selected the following values

$$\begin{aligned} \omega_k &= 100 + 100 \times k, & J_{\alpha,\beta} &= J = 10 \\ (k, \alpha, \beta &= 0, 1, 2, 3) & & \\ \omega &= (E_1 - E_0)/\hbar = 100 + 3J, & \Omega_k &= \Omega = 0.1. \end{aligned} \quad (14)$$

The characteristic parameters can be obtained multiplying (14) by 2π MHz. The selected frequency of the electromagnetic field, $\omega = (E_1 - E_0)/\hbar$, corresponds to the resonant transition $|0000\rangle \leftrightarrow |0001\rangle$. The time evolution of some reduced density matrix elements with our initial wavefunctions (11 a-d) is shown in figure 1(a-d).

We study the errors of the reduced density matrix elements as a function of the Rabi frequency, and the following different omegas from the $2\pi k$ method were chosen

$$\begin{aligned} \Omega_1 &= \frac{10}{\sqrt{4k^2 - 1}}, & \Omega_2 &= \frac{20}{\sqrt{4k^2 - 1}}, \\ \Omega_4 &= \frac{40}{\sqrt{4k^2 - 1}}. \end{aligned} \quad (15)$$

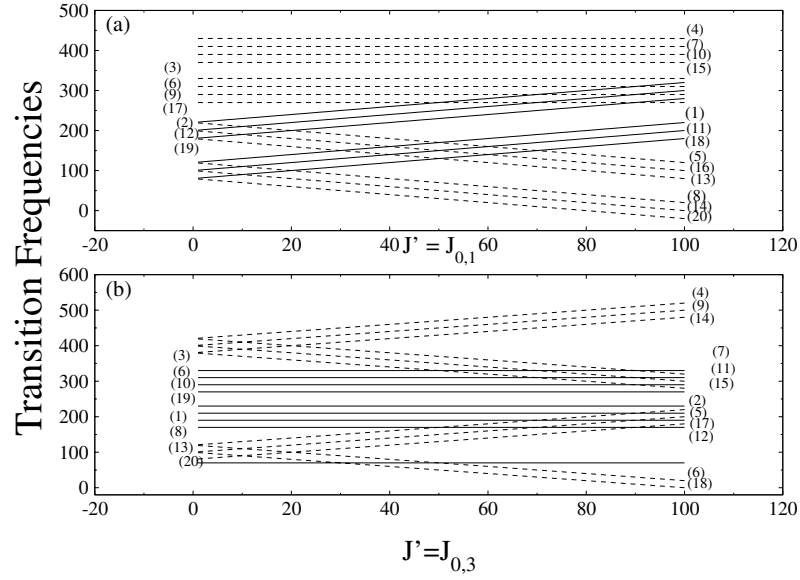


Figure 5. Variation of transition frequencies as a function of the coupling factor J' . (a) $J' = J_{01}$ and $J_{a,b} = J = 10$; and (b) $J' = J_{03}$ and $J_{a,b} = J = 10$. Line (1) represents the transition V_{01} and line (8) the transition $V_{2,3}$, the other labels represent transitions which are not relevant here.

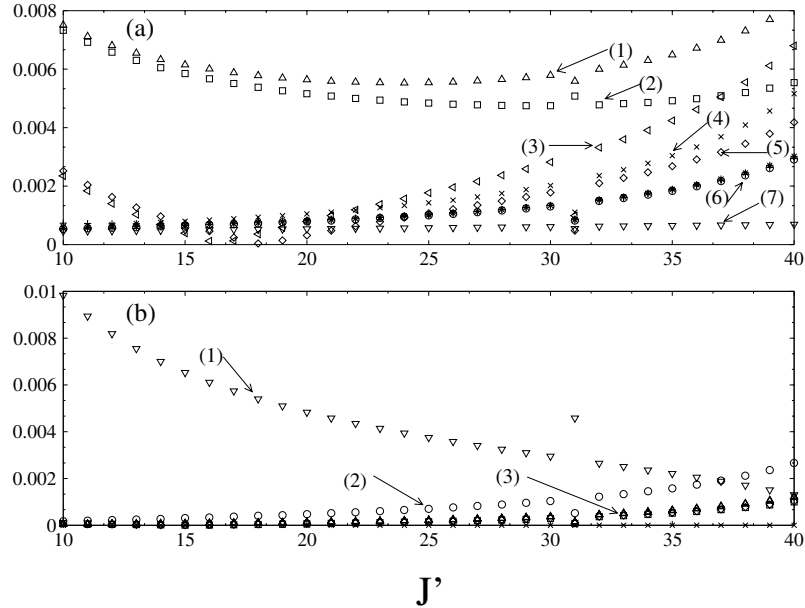


Figure 6. Variations of the real part of several density matrix elements as a function of the coupling parameters $J' = J_{01}$, fixing $J_{ab} = J = 10$, (1) $\text{Re } r_{22}$, (2) $\text{Re } r_{12}$, (3) $\text{Re } r_{23}$, (4) $\text{Re } r_{34}$, (5) $\text{Re } r_{13}$, (6) $\text{Re } r_{33}$, (7) $\text{Re } r_{24}$. (b) Variations of the imaginary part of several density matrix elements as a function of the same coupling parameters as (a), (1) $\text{Im } r_{33}$, (2) $\text{Im } r_{11}$, (3) $\text{Im } r_{22}$.

Ω_s was chosen in such a way that $\Omega_s = \Omega_1 = \Omega_2 = \Omega_4$ as shown in figure 2.

4. Results

We studied how the errors in the expected values of the reduced density matrix elements vary as a function of the Rabi frequency (Ω), having all the coupling constants equal to $J = 10$. This is shown in part (a) of figures 3 and 4, where just one matrix element is presented. Ω_s represents a Rabi frequency which is not selected from the $2\pi k$ method. To see which transition is responsible for the biggest contribution to the non-resonant effect and causes these errors, we eliminated

one matrix element of the interaction at a time and found that $V_{2,3}$ was the main factor responsible for these non-resonant transitions. Part (b) in figures 3 and 4 shows the error of the reduced density element $r_{2,3}$ at the end of the π -pulse for $V_{2,3} = 0$. We can see a drastic decrease in the value of this error.

Now, knowing that the resonant frequency for the transition $|2\rangle \leftrightarrow |3\rangle$ is given by $\omega_0 - J_{01} + J_{02} + J_{03}$, we select two different coupling constants J and J' to separate our resonant frequency $\omega_0 + J_{01} + J_{02} + J_{03}$ from this and other non-resonant frequencies. Choosing $J_{01} = J'$ and all the others with the same value, $J = J_{a,b} = 10$, $a \neq 0$, $b \neq 1$, we can get some separation as shown in part (a) of figure 5. If we choose $J_{03} = J'$ or $J_{02} = J'$ and all the other coupling

constants the same, $J = 10$, we do not get this separation, as can be seen in part (b) of figure 5. So, using $J_{01} = J'$ and all the other coupling constants the same, $J = 10$, we look for the variation of the errors on the expected values of the reduced density matrix elements as a function of this J' . This variation can be seen in figure 6. We found that the optimum value was $J' = 20$. In this way, using $J' = 20$, $J = 10$ and $V_{2,3} \neq 0$, we calculate the variation of the errors on the expected values of the reduced density matrix elements as a function of the Rabi frequency. This result can be seen in part (c) of figures 3 and 4.

5. Conclusions

Our numerical simulations show that the $2\pi k$ method with different coupling constants (as selected here) for the Ising interaction among spins properly suppresses the errors due to non-resonant transition for a quantum CN gate. Of course, this suppression does not mean that error corrections are no longer needed in quantum computation since other types of error and decoherence of the quantum system also need to be taken into account. On the other hand, this $2\pi k$ method can be applied to a very large number of qubits for a pure quantum system, as was shown by [22], who suggests that this method can also be applied to k -spin molecules with k much higher than four.

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